COMPUTER MODELING OF POLYMERS

by

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A Polymer Molecular Analysis Display System (p-MADS) was developed for computer modeling of polymers. This method of modeling allows for the theoretical calculation of molecular properties such as equilibrium geometries, conformational energies, heats of formations, crystal packing arrangements, and other properties. Furthermore, p-MADS has the following capabilities:

* Constructing molecules from internal coordinates (bonds lengths, angles, and dihedral angles), Cartesian coordinates (such as X-ray structures), or from stick drawings.
* Manipulating molecules using Graphics and to make hard copy representation of the molecules on a graphics printer.
* Performing geometry optimization calculations on molecules using the methods of Molecular Mechanics or Molecular Orbital Theory.

As shown in figure 1, p-MADS is a modular system consisting of four modules:

1. Main System (user module). This module links the other modules. User log into this module to extract information from one module and process it in another module.
2. Molecular Modeling System. Three dimensional structures are generated in the module for performing molecular operations such as rotation of molecules, comparision of two structures, and the examination of molecular distances.
3. Molecular Analysis System. The function of this module is to perform theoretical calculations on molecules.
4. Molecular Display System. This module outputs the information from the other modules to a printer or a graphics screen.

This particular design was chosen for p-MADS because it can be easily updated and readily adapted to new and improve hardware.

FIGURE 1. BLOCK DIAGRAM OF A POLYMER MOLECULAR ANALYSIS DISPLAY SYSTEM (p-MADS).